

Theory on Superconductivity of CeIn₃ in Heavy Fermion System

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On the basis of a three-dimensional Hubbard model, the superconducting mechanism of CeIn₃ under high pressure is investigated by the third-order perturbation theory with respect to the on-site Coulomb interaction U . Here we propose the d -wave pairing state induced by antiferromagnetic spin fluctuations. The estimated superconducting transition temperature is lower by one order than that in the two-dimensional system for the same value of U/W (W =bandwidth). This result is consistent with the difference between CeIn₃ and CeRhIn₅.

KEYWORDS: superconductivity, CeIn₃, CeRhIn₅, dimensionality, heavy fermion system, perturbation theory

Heavy fermion compound CeIn₃¹ has been confirmed to exhibit the properties of unconventional superconductivity. For instance, in the ¹¹⁵In-NQR measurement,² no coherence peak has been observed in the temperature dependence of $1/T_1$. The superconducting (SC) state appears under the pressure P with a critical value $P_c = 2.55$ GPa, and the maximum value of the SC-transition temperature $T_c^{\max} = 0.2$ K. The SC state exists near the antiferromagnetic (AF) phase with the ordering vector $Q = (\pi, \pi, \pi)$ at Ce atoms.³ The situation strongly suggests that superconductivity should be connected to three-dimensional (3D)-AF spin fluctuations.

In this paper, we assume that the CeIn₃ system is given by the Fermi liquid state at low temperatures and study the SC mechanism induced by the wave number dependence in the effective interaction between quasi particles originating from the Coulomb interaction among f -electrons. The SC state is considered to be realized on the main Fermi surface of Ce 4f-electrons.⁴ We pursue a possibility of the d -wave pairing state due to AF spin fluctuations near $\mathbf{Q} = (\pi, \pi, \pi)$. To describe the heavy fermions, here a 3D Hubbard model is adopted and the effective interaction is evaluated on the basis of the third-order perturbation theory (TOPT) in terms of the on-site Coulomb interaction^{5,6}. It is concluded that the SC mechanism of CeIn₃ is d -wave pairing induced by 3D-AF spin fluctuations near $\mathbf{Q}=(\pi, \pi, \pi)$.

In previous papers,^{7,8} two-dimensional (2D) and 3D single-band Hubbard models were generally investigated within fluctuation exchange approximation (FLEX). Although they treated different AF spin fluctuations depending on dimensions, they obtained the same result that T_c in the 3D system is lower than that in the 2D system. In addition to the characteristics of the AF spin fluctuation, we treated different wave number dependences due to the vertex correction in 2D and 3D dimensions.⁹

In this paper, we focus on CeIn₃ to discuss the microscopic mechanism of superconductivity. On the basis of TOPT, we investigate the effect of the interaction with the complex wave number dependence on the SC mech-

anism in 3D CeIn₃. The calculation based on TOPT includes also the normal self energy in this study of CeIn₃. We treat the wave number dependence originating from the main Fermi surface of CeIn₃ and the calculated T_c is reduced by renormalized Fermi energy E_F . As a result, we performed a new analysis of CeIn₃ in detail on the basis of TOPT. Next, we clarify the suppression of T_c by calculating the dependence of $T_c^{\text{TOPT}}/T_c^{\text{RPA-like}}$ on dimensionality. The change in T_c between 2D and 3D systems applies to that between 2D CeRhIn₅ and 3D CeIn₃. With regard to CeTIn₅ (T=Co, Rh and Ir), Takimoto, Hotta and Ueda¹⁰ studied the SC mechanism with a 2D orbital-degenerate Hubbard model. They indicated the appearance of the d -wave superconductivity next to the AF magnetic phase in the case where the crystal splitting energy is large. On the other hand, Nisikawa, Ikeda and Yamada¹¹ investigated the d -wave superconductivity in CeIr_xCo_{1-x}In₅ with the 2D single-band Hubbard model.

Here, we apply the single-band model to both CeIn₃ and CeRhIn₅ due to the following reason. The main Fermi surface of CeIn₃ is a single band as shown by the band calculation of Betsuyaku.⁴ The 3D single band induces the wave number dependence of the AF spin fluctuation, which plays the main role in superconductivity. Both CeIn₃ and CeRhIn₅ have the same kind of Ce compounds. Therefore, we apply TOPT to the superconductivity in the single band of CeRhIn₅ as well as CeIn₃. The main difference between the two materials is the dimensionality of the Fermi surface. We clarify the effect of dimensionality on the wave number dependence in the analysis based on TOPT, and moreover, we show the justification of the quasi-2D model in CeRhIn₅.

We explain the formulation in the following. The Hubbard Hamiltonian is given by

$$\mathcal{H} = -t_1 \sum_{\mathbf{i}, \mathbf{a}, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i+a}\sigma} + t_2 \sum_{\mathbf{i}, \mathbf{b}, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i+b}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}, \quad (1)$$

where $c_{\mathbf{i}\sigma}$ is an annihilation operator for a quasi particle with spin σ at site \mathbf{i} , \mathbf{a} and \mathbf{i} are, respectively, the vectors connecting nearest-neighbor and next-nearest-neighbor sites in a simple cubic lattice. Transfer integrals t_1 and t_2

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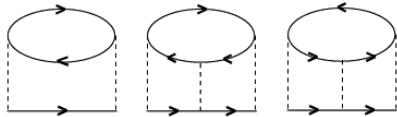


Fig. 1. Diagram of the normal self-energy $\Sigma_n(q, \omega_n)$. The solid line is the bare Green's function G_0 . The broken line is the Coulomb interaction U . The broken line of U connects only solid lines possessing opposite spins.

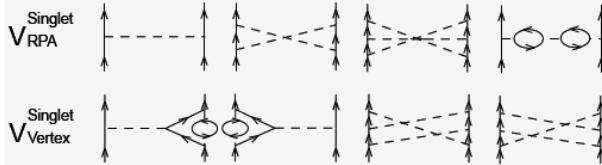


Fig. 2. Diagrams for the effective interaction of singlet pairing within the third-order perturbation with respect to U . The solid line is the bare Green's function G_0 . The broken line is the Coulomb interaction U . The broken line of U connects only solid lines possessing opposite spins. The two external lines have opposite spins. The effective interaction is divided into the RPA-like part and the vertex correction. The latter begins with the third-order terms.

denote nearest-neighbor and next-nearest-neighbor hopping amplitudes, respectively. U is the on-site Coulomb interaction, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. Here, we consider that the parameters t_1 , t_2 and U include a common renormalization factor¹¹ for constructing the heavy fermion. As shown in Fig. 3, we adjust the dispersion $E_{\mathbf{k}}$ so as to reproduce the main Fermi surface of heavy fermions constructed mainly by Ce 4f-electrons in the simple cubic structure,⁴ leading to

$$\begin{aligned} E_{\mathbf{k}} = & -2t_1(\cos k_x + \cos k_y + \cos k_z) \\ & + 4t_2(\cos k_x \cos k_y + \cos k_y \cos k_z + \cos k_z \cos k_x). \end{aligned} \quad (2)$$

Then, we obtain the bare Green's function of the quasi particle as $G_0(k) = 1/[i\omega_n - (E_k - \mu_0)]$, where k is a short-hand notation defined as $k = (\mathbf{k}, \omega_n)$, \mathbf{k} is momentum and $\omega_n = \pi T(2n + 1)$ is the fermion Matsubara frequency with temperature T . Note that the chemical potential μ_0 for the non-interaction case is determined by the electron number n (per site and spin) as $n = \sum_k G_0(k)$, where $\sum_k = (T/N) \sum_{\mathbf{k}} \sum_n$ and N is the number of sites. The dressed normal Green's function $G(k)$ is given by $G(k) = 1/[i\omega_n - (E_k - \mu) - \Sigma_n(k)]$, where $\Sigma_n(k)$ is the normal self-energy, given by TOPT with respect to U as

$$\Sigma_n(k) =$$

$$\sum_{k'} \{U^2 \chi_0(k-k') + U^3 [\chi_0^2(k-k') + \phi_0^2(k+k')] \} G_0(k'), \quad (3)$$

with

$$\chi_0(q) = - \sum_k G_0(k) G_0(q+k), \quad (4)$$

$$\phi_0(q) = - \sum_k G_0(k) G_0(q-k). \quad (5)$$

Here, q denotes a short-hand notation $q = (\mathbf{q}, \nu_n)$, where $\nu_n = 2\pi T n$ is the boson Matsubara frequency. Note that the chemical potential μ , shifted from μ_0 , is again determined by the condition $n = \sum_k G(k)$. We show the diagram of the normal self energy in Fig. 1.

An effective pairing interaction V between quasi particles is evaluated using TOPT. Although the origin of superconductivity is investigated by total terms in V , in order to analyze the role of V in detail, it is convenient to divide it into two parts as

$$V(k, k') = V_{RPA}(k, k') + V_{vertex}(k, k'), \quad (6)$$

where V_{RPA} represents the terms obtained by the random phase approximation (RPA) and V_{vertex} indicates the third-order vertex correction terms. The RPA-like term reflects the nature of simple spin fluctuations, while the third-order vertex correction terms originate from the electron correlation other than the spin fluctuations. For singlet pairing, V_{RPA} and V_{vertex} are given by

$$V_{RPA}(k, k') = U + U^2 \chi_0(k-k') + 2U^3 \chi_0^2(k-k'), \quad (7)$$

$$V_{vertex}(k, k') =$$

$$2U^3 \text{Re} \sum_{k''} G_0(k+k''-k') (\chi_0(k+k'') - \phi_0(k+k'')) G_0(k''). \quad (8)$$

We show the diagrams for singlet pairing in Fig. 2.

An anomalous self-energy Σ_a is expressed using $V(k, k')$ and an anomalous Green's function $F(k)$ as $\Sigma_a(k) = -\sum_{k'} V(k, k') F(k')$. At $T=T_c$, the linearized Eliashberg equation including Σ_a and $F(k)$ is reduced to the eigenvalue equation,

$$\lambda \Sigma_a^\dagger(k) = - \sum_{k'} V(k, k') |G(k')|^2 \Sigma_a^\dagger(k'). \quad (9)$$

When the eigenvalue λ becomes unity, the SC state is realized and T_c is obtained. We solve the equation on the assumption that Σ_a^\dagger has singlet or triplet pairing symmetry. We divide the first Brillouin zone into $64 \times 64 \times 64$ momentum meshes and take $N_f = 512$ for Matsubara frequency ω_n . The bandwidth W ($W^{3D} \sim 12t_1$) is a necessary range of ω_n for reliable calculations. The range is covered with the condition: $|W| < \pi T N_f$. To satisfy the condition, we calculate in the region with $T > 0.0037$.

As a result, the dominant symmetries are $d_{x^2-y^2}$ - and $d_{3z^2-r^2}$ -wave pairings, which are degenerate due to the space symmetry of the cubic system. In Fig. 4, we show the wave number dependence of the anomalous self-energy $\Sigma^A(q, \omega_n = \pi T)$ for $d_{x^2-y^2}$ -wave pairing. On the other hand, we did not obtain stable solution in the present calculations for other pairing symmetries such as d_{xy} -wave.

We explain in detail the mechanism of the d -wave pairing, which indicates $d_{x^2-y^2}$ or $d_{3z^2-r^2}$ -wave pairing. To describe the main large-volume Fermi surface⁴ (see Fig. 3), we choose a parameter set as $t_2 = -0.2$ and $n=0.45$, near the half-filling $n=0.5$. The main Fermi surface with a nesting property enhances the bare suscep-

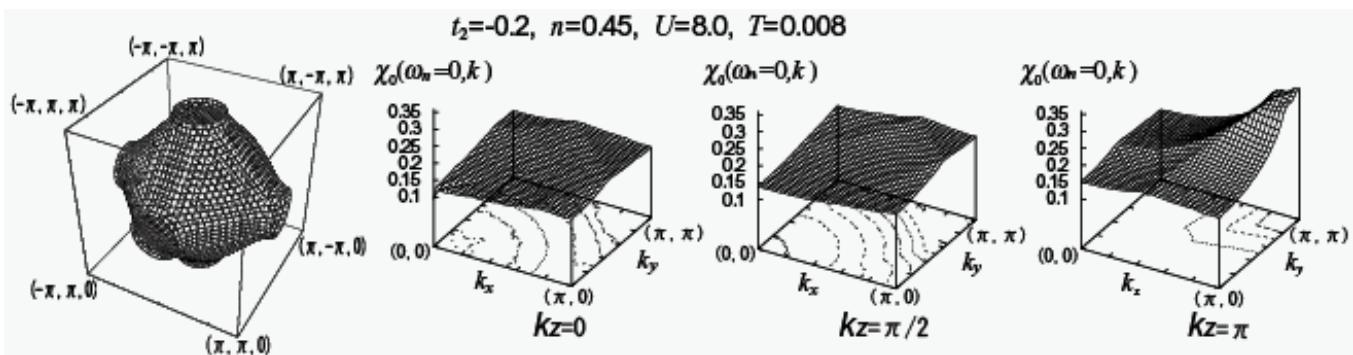


Fig. 3. Fermi surface in a quarter first Brillouin zone and bare susceptibility $\chi_0(q, \omega_n = 0)$.

tibility $\chi_0(\mathbf{q}, \nu_n)$, due to the feature of 3D-AF spin fluctuations near $\mathbf{Q}=(\pi, \pi, \pi)$, as shown in Fig. 3. The AF spin fluctuation originating from the RPA-like term provides an advantageous contribution to the eigenvalue λ for the d -wave pairing, as shown in Fig. 5. In the case including only the RPA-like terms, λ always increase with increasing U . However, it is significantly suppressed for a large U value when all terms in TOPT are taken into account, since the vertex correction terms suppress the d -wave superconductivity.

Next, we show the U dependence of T_c in Fig. 6. Here, it is emphasized that the evaluated T_c in the unit of t_1 is consistent with the experimental SC-transition temperature $T_c=0.2$ K in the value $T_c \sim 0.003$. We estimated the renormalized T_c with the electron effective mass m^* obtained by the experiment of dHvA. The details of the estimation are as the follows. The renormalized bandwidth W is given as zW_0 with the renormalization factor z . As another relation, W is given as $W=12t_1$ from the $t_2=-0.2$. Here, W_0 is a bare bandwidth. The renormalization factor is defined by $z=m_0/m^*$ and m_0 is the bare electron mass. dispersion $E_{\mathbf{k}}$ of eq. (2) at . Therefore, the relation of W is $12t_1=zW_0$. The bare bandwidth W_0 is $W_0 \sim 0.1$ Ry=1.58 $\times 10^4$ K in the band calculation.⁴ z is obtained as $z=1/16$ using the cyclotron mass of dHvA.¹² From the relation, the renormalized t_1 is obtained as $t_1=0.819 \times 10^2$ K. By means of t_1 , the calculated value $T_c \sim 0.003(t_1)$ at $U \sim 9.0$ corresponds to $T_c=0.246$ K, which is near the experimental SC-transition temperature $T_c=0.2$ K. Thus, the present calculation for T_c well explains the possibility of the d -wave pairing state in CeIn₃. Because the calculated T_c on the basis of TOPT is near the experimental SC-transition temperature, we consider that the system has a strong electron correlation $U \sim 9.0$, which is larger than the value of the bandwidth.

Furthermore, it is quite instructive to consider the comparison between 2D and 3D cases. We investigate the effect of dimensionality on the constant strength of the substantial electron correlation. Here, the strength of the substantial electron correlation means the value of U in comparison with the bandwidth. Thus, U/W keeps a constant value in the change from 2D to 3D systems. For the same value of $U/W \sim 3/4$ ($t_2=-0.2$, $n=0.45$, $W^{3D} \sim 12t_1$ and $W^{2D} \sim 8t_1$), we obtain $T_c^{2D}=0.042$

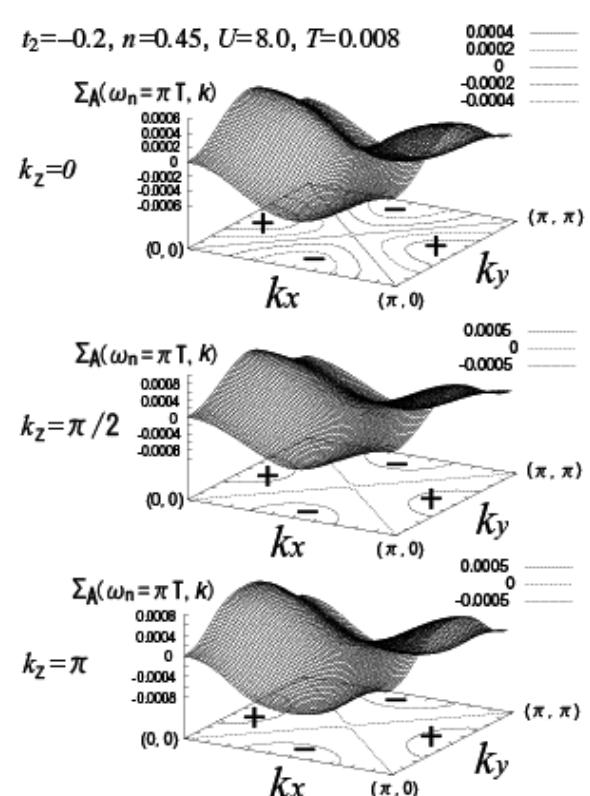


Fig. 4. Anomalous self-energy $\Sigma^A(q, \omega_n = \pi T)$ for $d_{x^2-y^2}$ -wave pairing.

in a 2D square lattice and $T_c^{3D}=0.0067$ in a 3D simple cubic lattice. Namely, T_c for the 3D system is lower by about one order than that for the 2D system. This is consistent with the experimental findings that $T_c^{3D} \approx 0.2$ K for CeIn₃ (3D system) and $T_c^{2D} \approx 2.1$ K for CeRhIn₅ (quasi-2D system).¹³

We show in Fig. 7 the change in $T_c^{\text{TOPT}}/T_c^{\text{RPA}}$ between 2D and 3D systems obtained by the present calculation using the dispersion

$$\begin{aligned} E_{\mathbf{k}} &= -2t_1(\cos k_x + \cos k_y + t_z \cos k_z) \\ &+ 4t_2(\cos k_x \cos k_y + t_z \cos k_y \cos k_z + t_z \cos k_z \cos k_x). \end{aligned} \quad (10)$$

Here, the hopping integrals t_1 and t_2 in the c-axis direction are multiplied by t_z . Namely, the dispersion relations with $t_z=0$ and 1 correspond to those for the 2D square and 3D simple cubic lattices, respectively. As a result, the suppression of T_c by the vertex correction is stronger

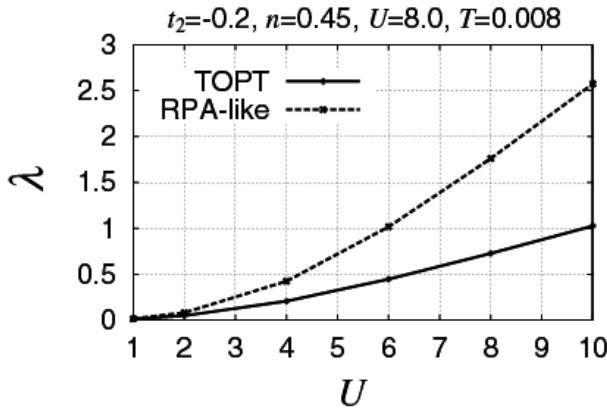


Fig. 5. U dependence of the eigenvalue λ obtained by TOPT and RPA-like terms.

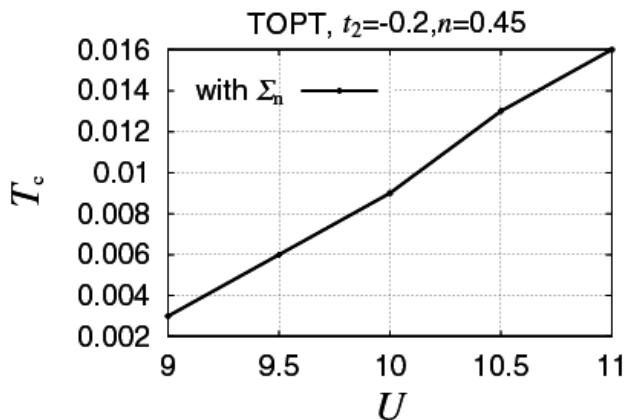


Fig. 6. U dependence of T_c calculated by TOPT.

in the 3D system than in the 2D system. By including the suppression on the basis of TOPT, the difference in T_c becomes one order between 2D and 3D systems. In addition to this, the decrease in T_c is slight with the increase in the 3D characteristic in the region near the quasi-2D system. Actually, in the range that t_z is small ($t_z = 0 \sim 0.4$), the change in T_c by TOPT is small under the condition that U/W is constant (see the inset of Fig. 7). Therefore, the T_c calculated on the basis of the 2D model is appropriate for CeRhIn₅, even if the band structure of CeRhIn₅ possesses a weak 3D characteristic.

Here, we explain the different suppression depending on dimensionality in the analysis of TOPT. We consider the wave number dependence of χ_0 on the k_x-k_y plane perpendicular to the k_z -axis, as shown in Fig. 3. In the quasi-2D system with AF spin fluctuations, the same prominent peaks exist near $Q=(\pi, \pi)$ on planes at all k_z . In the 3D system, χ_0 has prominent peaks around $Q=(\pi, \pi)$ on planes only near $k_z=\pi$. On the other hand, since the prominent peaks exist on planes at all k_z in the quasi-2D system, the RPA-like term naturally gives high T_c in the quasi-2D system rather than in the 3D system. This fact has been known in previous studies.^{7,8,14} On the other hand, the complex wave number dependence exists except for the region around Q . As opposed to the prominent peaks, the momentum space possessing the

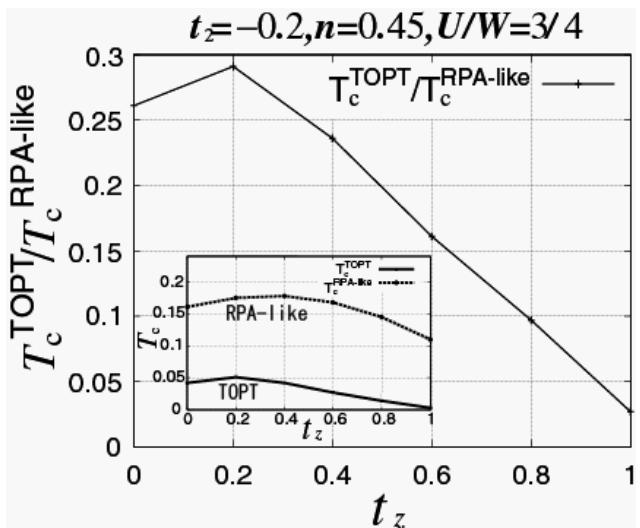


Fig. 7. Change in $T_c^{\text{TOPT}}/T_c^{\text{RPA}}$ between 2D and 3D systems at the same value of W/U . The inset shows T_c^{TOPT} and $T_c^{\text{RPA-like}}$ obtained by TOPT and RPA-like calculations.

complex wave number dependence occupies a larger region in the 3D system than in the quasi-2D system. For example, in the 3D system, the complex wave number dependence spreads on planes at $k_z = 0$ and $\pi/2$ in Fig. 3. Therefore, the suppression by the vertex correction in the 3D system is stronger than that in the quasi-2D system. In addition to the characteristics of the AF spin fluctuation, we obtain T_c by including the effect of the complex wave number dependence in TOPT. The calculated T_c is near to the realistic SC-transition temperature by including each wave number dependence for each dimensional system. Therefore, we compare the T_c obtained by TOPT with the experimental SC-transition temperature in CeIn₃ and CeRhIn₅.

We summarize our study of the superconductivity in CeIn₃. By means of TOPT based on the 3D Hubbard model, we explained the mechanism of the superconductivity of CeIn₃ from a microscopic point of view. It is concluded that the SC mechanism of CeIn₃ is $d_{x^2-y^2}$ (or $d_{3z^2-r^2}$ -wave) pairing, mainly induced by 3D-AF spin fluctuations near $Q=(\pi, \pi, \pi)$. In the present calculation including the suppression of T_c by the third-order vertex correction, T_c in the 3D cubic systems is lower by one order than that in the 2D square system for the same value of U/W , in good agreement with the experimental results for 2D and 3D Ce-based heavy fermion superconductors, CeRhIn₅ and CeIn₃. It has been pointed out by means of FLEX that the superconductivity induced by AF spin fluctuations is suppressed in the 3D system compared with that in the 2D system^{7,8} but here we stress that the difference is obtained also by means of TOPT including the vertex correction in this paper. Moreover, we found that the suppression of T_c by the vertex correction is stronger in the 3D system than in the 2D system for the same value of U/W . A part of this paper is contained in the proceeding of ASR2002.¹⁵ The authors thank Dr. H. Ikeda, Professo T. Hotta and Professor H. Harima for valuable discussions.

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